

Dynamical Correlations as Origin of Nonextensive Entropy

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Abstract

We present a simple and general argument showing that a class of dynamical correlations give rise to the so-called Tsallis nonextensive statistics. An example of a system having such a dynamics is given, exhibiting a non-Boltzmann energy distribution. A relation with prethermalization processes is discussed.

1 Generalized statistics and correlations

In the recent paper by J. Berges et al. [1], the authors show that the dynamics of a quantum scalar field exhibits a prethermalization behavior, where the thermodynamical relations become valid long before the real thermal equilibrium is attained. There, although the system is spatially homogeneous, the single particle spectra are different from those determined by the usual Boltzmann equilibrium. This means that the validity of thermodynamics does not imply thermal equilibrium in the sense of Boltzmann.

Such a situation has also long been claimed by Tsallis [2, 3], who introduced the q -entropy, defined in terms of the occupation probabilities $\{p_\alpha\}$ of the microstate α by

$$S_q[\{p_\alpha\}] = \frac{1 - \sum_\alpha p_\alpha^q}{q - 1}, \quad (1)$$

instead of the usual entropy $S[\{p_\alpha\}] = -\sum_\alpha p_\alpha \ln p_\alpha$. All thermodynamical relations are derived from the maximization of this q -entropy,

$$\delta S_q - \frac{1}{T} \delta \langle E \rangle_q + \lambda \delta \sum_\alpha p_\alpha = 0, \quad (2)$$

where

$$\langle E \rangle_q = \frac{\sum_\alpha p_\alpha^q E_\alpha}{\sum_\alpha p_\alpha^q} \quad (3)$$

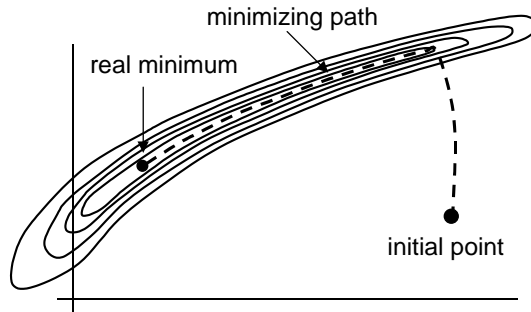


Figure 1: Schematic illustration of the effect of a strong correlation among two variables for minimizing a function.

is the q -biased average of the energy. It is shown that, although the thermodynamical Legendre structure is maintained, the energy spectrum for such a system is not given by Boltzmann statistics but behaves asymptotically like a power in E [2, 3]. In other words, the thermal equilibrium in the sense of Boltzmann is a sufficient condition, but not a necessary one for the thermodynamic relations to be valid. Extensive studies have been developed [3] and the applications of Tsallis' entropy extend to biological systems, high-energy physics, and cosmology. However, in spite of these studies, the dynamical origin of the q -entropy and q -biased average of observables is not clear yet.

It has been suggested that Tsallis' nonextensive statistics applies to a kind of metastable state which is realized before the true thermal equilibrium, or to some stationary state having long-range correlation [3]. This is exactly another important result of J. Berges et al., that their preequilibrium state is attained long before the real equilibrium is reached, that is, the system seems to attain first this preequilibrium, then slowly goes to the real equilibrium. This reminds us somewhat of the following situation which we encounter frequently in optimization problems. For example, let us consider the problem of finding a minimum of a function of two variables, as shown in Fig. 1.

When the function has a narrow long valley, the usual steepest descent method always first goes to the closest point of the valley instead of going directly to the real minimum, as indicated by the dashed curve. The narrow valley means that there exists a strong correlation between the two variables. In other words, if there exist any strong correlations among variables, the minimizing path always tries to satisfy the correlation first, then follows downstream to the true minimum along the valley generated by the correlation. If the correlation is strong enough, non Boltzmann distribution may result as the stable configuration of the system (see Ref. [5]).

The above consideration suggests that a preequilibrium state may correspond to a kind of narrow valley of the free energy of some subsystem generated by dynamical correlations of the system. If such a local minimum stays for a very

long time, we may consider the system as in equilibrium, but the microscopic occupation probability is not that of the Maxwell-Boltzmann distribution. Then what characterizes such a local equilibrium? We suggest here that a general form of Tsallis' statistics is one answer. Of course, prethermalization involves a broad range of phenomena, and has been studied for a long time in several works (for recent references, see [4]). Here we concentrate on the discussion of how the states described by the Tsallis nonextensive statistics can be regarded as a kind of prethermalized states.

Let us consider a system composed of N particles and let $\{E_\alpha\}$ denote the single-particle spectrum of the system and $\{N_\alpha\}$ be the corresponding occupation numbers. We further assume that the system is dilute enough that the interaction energies are negligible. Then, by definition, $E = \sum_\alpha N_\alpha E_\alpha$ and $N = \sum_\alpha N_\alpha$ are, respectively, the total energy and total number of particles of the system. Suppose there exists a strong correlation among any q particles of N_α in any single-particle state α . Then the number of possible ways of forming such correlated subsystems in each α state is given by

$$M_\alpha = \binom{N_\alpha}{q} \approx \frac{N_\alpha^q}{\Gamma(q+1)} \quad (4)$$

for $N_\alpha \gg q$. Note that here, q does not have to be integer. We call these correlated systems q -clusters. The total number of ways of forming q -cluster states for the whole system is

$$M = \sum_\alpha M_\alpha. \quad (5)$$

If the q -clusters are formed with equal a priori probability, thus proportional to the number of ways of forming them, then the average energy per cluster particle is

$$\langle E \rangle_q = \frac{\sum_\alpha M_\alpha E_\alpha}{\sum_\alpha M_\alpha} = \frac{\sum_\alpha p_\alpha^q E_\alpha}{\sum_\alpha p_\alpha^q}, \quad (6)$$

where $p_\alpha = N_\alpha/N$ is the probability of a particle occupying state α .

Now, we further assume that the dynamical evolution of the system is such that, for a given number of q -clusters, the configuration of the system tries to minimize the energy of the correlated subsystem. That is, for some arbitrary initial condition, the system first generates correlations among particles in such a way to minimize the energy in the clusters. The narrow valley in Fig. 1 corresponds to these "ground states" of the subsystem formed by q -clusters. Neglecting the component perpendicular to the narrow valley, the equilibrium corresponds to minima of the expectation value $\langle E \rangle_q$,

$$\delta \langle E \rangle_q = 0, \quad (7)$$

under the conditions

$$\sum_{\alpha} N_{\alpha} = N, \quad (8)$$

$$\sum_{\alpha} p_{\alpha}^q = \frac{M}{N^q} = A = \text{const}. \quad (9)$$

This is equivalent to the variational problem,

$$\delta \left[\frac{\sum_{\alpha} p_{\alpha}^q E_{\alpha}}{\sum_{\alpha} p_{\alpha}^q} + \lambda \left(\sum_{\alpha} p_{\alpha}^q - A \right) + \nu \left(\sum_{\alpha} p_{\alpha} - 1 \right) \right] = 0, \quad (10)$$

which determines the probabilities p_{α} . We obtain:

$$p_{\alpha} = \frac{1}{Z_q} \left[1 + \frac{1}{\lambda A} (E_{\alpha} - \langle E \rangle_q) \right]^{1/(1-q)}, \quad (11)$$

where $Z_q = A^{1/(1-q)}$ is a normalization factor. We see that this expression is nothing but the Tsallis distribution function, if we put $\lambda^{-1} = (q-1)\beta$. Note that there was no need to introduce the concept of entropy yet. The Tsallis entropy here corresponds to the simple normalization condition for the number of q -clusters.

It is important to note that the minimization condition, Eq.(10), of the energy of the correlated subsystems under the constraint Eq.(9) determines completely the occupation probabilities for the whole system as functions of A and of the single-particle spectrum, $p_{\alpha} = p_{\alpha}(A, \{E_i\})$. When we change the external parameters of the system, such as the volume V , then the single-particle spectrum will suffer a change. However, if the dynamics of the system is such that the number of correlated particles q is kept constant during slow changes of V and N , then we can consider V , N , and A independent “state” parameters, since the occupation probabilities for the system are completely determined by these variables. We can thus calculate the total energy as function of them as

$$E(V, A, N) = N \sum_{\alpha} p_{\alpha} E_{\alpha}. \quad (12)$$

Comparing the variation of this energy function with the First Law of Thermodynamics, $\delta E = -P\delta V + T\delta S + \mu\delta N$, we can identify the pressure

$$P = -N \sum_{\alpha} \left(\sum_{\beta} \left(\frac{\partial p_{\beta}}{\partial E_{\alpha}} \right)_A E_{\beta} + p_{\alpha} \right) \frac{\partial E_{\alpha}}{\partial V}, \quad (13)$$

the chemical potential $\mu = \sum_{\alpha} p_{\alpha} E_{\alpha}$, and the entropy term

$$T\delta S = \left[N \sum_{\alpha} \left(\frac{\partial p_{\alpha}}{\partial A} \right)_V E_{\alpha} \right] \delta A. \quad (14)$$

Eq. (14), implies that we can relate the parameter A to the entropy of the system, up to an arbitrary function $f(A)$,

$$S = f(A), \quad (15)$$

and have a temperature given by

$$T = \frac{1}{f'(A)} \left[\sum_{\alpha} \left(\frac{\partial p_{\alpha}}{\partial A} \right)_V E_{\alpha} \right]. \quad (16)$$

If we take $f(A) = \ln A / (1 - q)$, then

$$S = \frac{\ln(\sum_{\alpha} p_{\alpha}^q)}{1 - q} \quad (17)$$

is the Renyi entropy. If instead we take $f(A) = (A - 1)/(1 - q)$, S corresponds exactly to the Tsallis entropy (1). This indeterminacy is obvious also from Eq. (10), since the constraint term $\lambda(\sum p_{\alpha}^q - A)$ can also be taken as $\lambda'[f(\sum p_{\alpha}^q) - f(A)]$ without changing its significance, for any single-valued function f . Thus, it is clear that the exact form of f is not essential in our approach.

We should stress that the thermodynamical properties of the preequilibrium state discussed above are not the nonextensive ones discussed by Tsallis et al. [2, 3]. There, the thermodynamical and statistical properties for q -modified values are studied. In the present approach, the q -modified quantities refer to the subsystem of q -clusters. When we want to calculate, for example, the internal energy of the system, the relevant quantity is not $\langle E \rangle_q$ but just the usual total energy E . Therefore, the effective equation of state, that is, the relation between pressure and energy density given by Eq. (13), will apply immediately as the real physical relation which can be used, for example, in hydrodynamical calculations. However, the “entropy” here is not the real entropy of the whole system but just reflects the total number of clusters among correlated particles. Thus, the time evolution of this quantity is not guaranteed to obey the Second Law of Thermodynamics, that is, $dS/dt \geq 0$. Hereafter, in order to distinguish from the real entropy, we call this S the “pseudo-entropy” of the total system.

On the other hand, note that the variational equation Eq. (10) can also be obtained as that of maximizing the cluster multiplicity M at a fixed average energy per cluster. We would have the variational equation,

$$\delta \left[M + \beta (\langle E \rangle_q - E_C) + \nu \left(\sum_{\alpha} p_{\alpha} - 1 \right) \right] = 0, \quad (18)$$

where E_C is the average energy per cluster, and β and ν are Lagrange multipliers. This leads to the same equation as Eq. (10). Since M is the total number of possible ways to form clusters, we can define the “entropy” of the system of clusters by $S_q = \ln M$, and this corresponds to the Renyi entropy, Eq. (17). Therefore, Eq. (10) is nothing but the maximization of the entropy defined only

for the restricted subspace corresponding to the degrees of freedom of clusters in the entire phase space of the system.

In the above discussion, we considered the value of q , i.e., the number of strongly correlated particles as constant for any single-particle state α . However, in a more general case, they may be different for each single-particle state and may even depend on the proper occupation numbers p_α . Therefore, for a more general form of the correlation pattern, the number of cluster states M_α should be written as

$$M_\alpha = M_\alpha[\{p_\alpha\}] = \frac{p_\alpha^{F_\alpha[\{p_\alpha\}]}}{\Gamma(F_\alpha[\{p_\alpha\}] + 1)} \quad (19)$$

where $F_\alpha[\{p_\alpha\}]$ are functionals of $\{p_\alpha\}$. Then, the Eq. (10) should have the form

$$\delta \left[\frac{\sum M_\alpha[\{p_\alpha\}] E_\alpha}{\sum M_\alpha[\{p_\alpha\}]} + \lambda \left(\sum M_\alpha[\{p_\alpha\}] - M \right) + \nu \left(\sum p_\alpha - 1 \right) \right] = 0. \quad (20)$$

The resulting probabilities p_α will not be of the form of Eq. (11) anymore, yet functions of V , N , and M . This suggests that the preequilibrium state can be attained for a wide variety of single-particle spectra and the corresponding pseudo-entropy will be given as a function of M , $S = f(M) = f(\sum_\alpha M_\alpha)$. This is presumably the most general form of the pseudo-entropy. However, we should recall that it does not necessarily possess the properties of entropy required by the usual thermodynamics because the state specified by Eq.(20) does not correspond to the conventional equilibrium of the system.

2 Example

Discussion in the previous section indicates what kind of dynamical correlations may lead to Tsallis type occupation probability distribution. Just to see a concrete example let us consider a very simple toy model described below.

1. Initially N particles are distributed as $\{N_0, N_1, \dots, N_\alpha, \dots\}$ over equally spaced energy levels. Let us denote the energy of the i -th particle as E_i .
2. Choose randomly a pair of particles, say, i and j .
3. Energies of i and j are updated according to one of the following alternatives:
 - (a) The new energies are set to the lower one of E_i and E_j , that is, $E_i, E_j \rightarrow E'_i = E'_j = \text{Min}(E_i, E_j)$, then choose another k -th ($k \neq i, j$) particle randomly and attribute $E'_k = E_k + \text{Max}(E_i, E_j) - \text{Min}(E_i, E_j)$ to conserve the total energy.
 - (b) Change the energies as $E_i \rightarrow E'_i = E_i \pm \Delta E$ and $E_j \rightarrow E'_j = E_j \mp \Delta E$, where ΔE is the level spacing. Here, if one of E'_i, E'_j becomes negative, then this step is skipped. That is, we have to keep always $E_i \geq 0$.

4. The alternatives (a) and (b) are chosen randomly, but the ratio of the average frequency of (a) to (b) is kept as a constant, r .

It is well-known that for $r = 0$ in the above model, the ultimate single-particle spectrum will be the Boltzmann distribution. When $r > 0$, the collisions of type (a) are forming a kind of cluster, while the collisions of type (b) may destroy a correlation formed before. Thus, we expect the number of correlated particles will reach some stationary value. Furthermore, by construction, the energy of a correlated pair always tends to diminish. In this way, we may expect that the above system will lead to the situation described by Eq. (10). In Fig. 2, we show the results of simulations, for several values of r from 0.00001 to 0.1. It is interesting to note that $r > 0$ leads to a non-Boltzmann distribution which is well approximated by the Tsallis distribution, $p_a = C/[1 + (q - 1)\beta E_\alpha]^{1/(1-q)}$, where $\beta = 1/(3 - 2q)\langle E \rangle$ and $C = (2 - q)/(3 - 2q)\langle E \rangle$ are determined from the normalization condition and conservation of energy. One parameter fits with respect to q were performed and the results are indicated by the continuous curves in this figure. For $r \rightarrow 0$, the spectrum converges to the Boltzmann distribution $p_a \rightarrow e^{-E_\alpha/\langle E \rangle}$ as expected. Note that for a one dimensional case like the present model, the Tsallis distribution is valid only for $q < 3/2$, otherwise the energy expectation value diverges. For larger values of r , the fitted value of q tends to this limiting value, but the distribution begins to deviate substantially from the Tsallis distribution in the low energy region.

It is important to note that these distributions are the stationary and stable ones. We confirm that starting from any different initial conditions, the system always converges to the same final distribution, uniquely determined by the r parameter. Furthermore, the convergence for $r > 0$ is much faster than for $r = 0$. For example, taking $r = 0.01$ we find that the distribution converges 10 times faster than for $r = 0$.

In the above toy model, time reversal is violated in type (a) collisions. However, this is not the crucial factor to obtain the non-Boltzmann distribution. We have checked this in a more elaborate model which has time-reversal invariance.

3 Conclusions and perspectives

We have shown that a very simple mechanism of dynamical correlations among particles may lead to a state described by the so-called nonextensive statistics of Tsallis. It is shown that the nonextensive statistics can be interpreted as the statistical mechanics for a subspace defined by these strongly correlated clusters in the entire phase space of the whole system. Furthermore, the requirement of the minimum energy per cluster or the maximum “entropy” of the subspace defines the thermodynamical properties of the whole system too. There, the energy is defined by the usual sum of single-particle energies multiplied by their occupation probability, and not by the q -weighted average of the energy. We have also shown a toy model for which such a mechanism actually takes place.

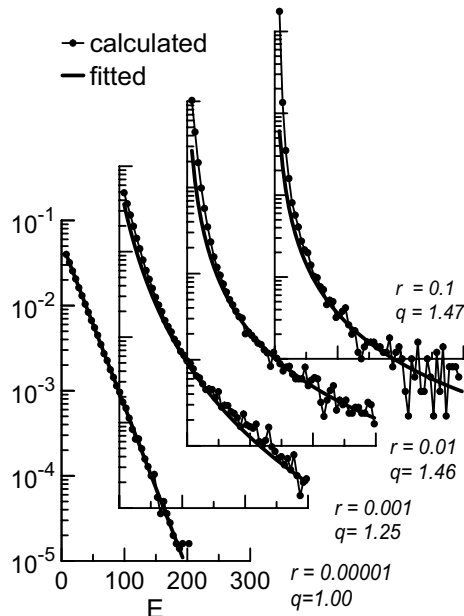


Figure 2: Energy spectrum after a large number of collisions per particle, starting from a distribution peaked at $\langle E \rangle = 22.5$. The probability of cluster-forming collisions ranges from $r = 0.1$ (top) to $r = 0.00001$ (bottom). Tsallis distributions fitted to the calculated spectra are also shown, together with the corresponding q -values.

In this example, the stationary state is attained with a single-particle spectrum which is well represented by that of Tsallis statistics. These stationary non-Boltzmann distributions are attained much earlier than the case of no correlations, hence the Boltzmann equilibrium. The reason for reaching the stationary distribution much earlier than the real thermal equilibrium is that the formation of correlated clusters serves as a kind of catalyzer to distribute the energy among particles more efficiently, involving more than 2-body collisions. In this aspect, the dynamical mechanism responsible for the non-Boltzmann distribution is similar to that of the kinematical approach discussed by Rafelski et al. [6]. Many examples of systems for which Tsallis statistics have been applied may also be interpreted in our scheme easily. We also found that this non-Boltzmann equilibrium may happen not only with a power type but with a much wider class of single-particle spectra.

The present work is rather phenomenological and so the conclusion is still speculative. More theoretical work based on realistic field theoretical models should be developed. Further investigations in this line are in progress. This work has been supported by CNPq, FINEP, FAPERJ, and CAPES/PROBRAL.

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